XAI FOR WINE QUALITY CLASSIFICATION USING SHAPLEY ADDITIVE EXPLANATIONS IN INTERPRET FEATURE IMPORTANCE IN SUPERVISED LEARNING

FINAL THESIS

IHSANUL ARIFIN RAMADHANI
41522010249

INFORMATICS ENGINEERING STUDY PROGRAM

FACULTY OF COMPUTER SCIENCE

INTERNATIONAL UNDERGRADUATE PROGRAM

MERCU BUANA UNIVERSITY

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SUBMITTED AS ONE OF THE REQUIREMENTS FOR PRESENTATION AT THE FINAL THESIS DEFENSE

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MOTTO & ACKNOWLEDGEMENTS

Whatever progress I have made rests upon the quiet sacrifices of my closest people. Their steadfast resilience and unspoken support have shaped my path, and this thesis stands as a testament to the values they have lived, perseverance, humility, and unwavering devotion.

First and foremost:

1. To my beloved parents Mum and Dad, Rina Sumarni and Yusya Januar, I dedicate this thesis to you. You carried what I did not see, endured what you rarely spoke of, and kept going when it would have been easier to stop. Your love was not loud, but it was constant, not performative, but steadfast. If there is any strength in these pages, it is because I learned endurance from you quietly, over time, through the way you lived.
2. To my partner, Ditha Firsty Auguestien, thank you for being my steadier horizon throughout this journey. For the patience in the long seasons of work, the kindness in moments of doubt, and the gentle reminders to keep going when I felt spent, your support has mattered more than you know. This thesis carries, between its lines, the calm you gave me when I needed it most
3. To the lecturers of the International Undergraduate Informatics Engineering Programme at Universitas Mercu Buana, I extend my sincere appreciation. Thank you for the discipline you upheld and the knowledge you entrusted to your students. You shaped not only what I know, but how I think, how I question, refine, and pursue clarity with rigour.
4. I would also like to express my sincere gratitude to my supervisor, Ilham Nugraha, S.Kom., M.Sc., for his guidance, constructive feedback, and steady support throughout the thesis process. His suggestions helped sharpen both the direction of the research and the clarity of its presentation, and his supervision made this work far more structured and achievable.

5. To my coursemates four companions from the same cohort and programme Joao Nitoivar Ribeiro Cancio, David Ginola Guterres, Muhammad Ilham Haekal, and M. Chandra Agoeng Pramudya Abdullah thank you for the camaraderie that carried me through ordinary weeks and difficult deadlines alike.
6. My thanks also go to my friends from my daily circle Rais Khan, Muhammad Mahrus Irsyam, and Hamzah Nuriadi for the encouragement, humour, and companionship that kept me grounded.
7. I am also grateful to the places that became part of my routine and, in their own way, part of this thesis. Thank you to Madurani, which at times offered a reliable corner for drafting and revising, and to Bu'de and the warmth of that small shop environment that made working there feel welcoming. My appreciation also extends to Kopi Kenangan, which often became my workspace for revisions and long writing sessions.
8. And, on a lighter note, I would like to thank the craft of coffee itself especially espresso, Americano, latte, and aren latte which became reliable fuel through long hours of analysis, coding, and writing.
9. Last but not least, I wanna thank me for believing in me, I wanna thank me for doing all this hard work. I wanna thank me for having no days off. I wanna thank me for never quitting. I wanna thank me for always being a giver and trying to give more than I receive. I wanna thank me for trying to do more right than wrong. I wanna thank me for being me at all times.

ABSTRACT

Name : Ihsanul Arifin Ramadhani

Student ID : 41522010249

Study Program : Undergraduate Informatics Engineering Programme

Title of Research : *XAI for Wine Quality Classification Using Shapley Additive Explanations in Interpreting Feature Importance in Supervised Learning*

Supervisor : Ilham Nugraha, S.Kom., M.Sc.

This study investigates explainable supervised learning for red wine quality classification using the UCI Wine Quality (red wine) dataset (1,599 samples; 11 physicochemical features). The ordinal quality score is converted into a binary label (quality ≤ 5: low; quality ≥ 6: high). Using an 80/20 stratified split, Logistic Regression, Random Forest, and XGBoost are compared, with F1-score as the primary metric. XGBoost delivers the best held-out test performance, achieving F1 = 0.8452 at the default 0.50 threshold. A single global decision threshold is then selected from out-of-fold probabilities via stratified cross-validation on the training set, avoiding test-set tuning. The optimal threshold of 0.45 yields a modest improvement on the test set (F1 = 0.8487) with slightly higher recall. SHAP explanations show that alcohol and sulphates typically raise high-quality likelihood, while volatile acidity and total sulphur dioxide push predictions towards low quality. These findings support accurate yet transparent quality screening.

Keywords: Explainable AI, SHAP, XGBoost, supervised learning, wine quality classification, threshold calibration, feature importance.

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ABSTRAK

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Judul Penelitian : *XAI for Wine Quality Classification Using Shapley Additive Explanations in Interpreting Feature Importance in Supervised Learning*

Pembimbing : Ilham Nugraha, S.Kom., M.Sc.

Studi ini meneliti penerapan *explainable supervised learning* untuk klasifikasi kualitas red wine menggunakan dataset UCI Wine Quality (red wine) (1.599 sampel; 11 fitur fisikokimia). Skor kualitas ordinal dikonversi menjadi label biner (kualitas ≤ 5: rendah; kualitas ≥ 6: tinggi). Dengan *stratified split* 80/20, Logistic Regression, Random Forest, dan XGBoost dibandingkan, dengan F1-score sebagai metrik utama. XGBoost memberikan kinerja terbaik pada *held-out test set*, mencapai F1 = 0,8452 pada ambang (threshold) default 0,50. Selanjutnya, satu ambang keputusan global dipilih dari probabilitas *out-of-fold* melalui *stratified cross-validation* pada data latih, sehingga menghindari penyesuaian ambang pada data uji. Ambang optimal 0,45 menghasilkan peningkatan kecil pada data uji (F1 = 0,8487) dengan recall yang sedikit lebih tinggi. Penjelasan SHAP menunjukkan bahwa alkohol dan sulphates umumnya meningkatkan peluang kualitas tinggi, sedangkan *volatile acidity* dan *total sulphur dioxide* mendorong prediksi ke kualitas rendah. Temuan ini mendukung penyaringan kualitas yang akurat sekaligus transparan.

Kata Kunci: Explainable AI, SHAP, XGBoost, supervised learning, wine quality classification, threshold calibration, feature importance.

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